

# Hole-pair symmetry and excitations in the strong-coupling extended $t - J_z$ model: competition between $d$ -wave and $p$ -wave

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We analytically calculate the ground state pairing symmetry and excitation spectra of two holes doped into the half-filled  $t - t' - t'' - J_z$  model in the strong-coupling limit ( $J_z \gg |t|, |t'|, |t''|$ ). In leading order, this reduces to the  $t' - t'' - J_z$  model, where there are regions of  $d$ -wave,  $s$ -wave, and (degenerate)  $p$ -wave symmetry. We find that the  $t - J_z$  model maps in lowest order onto the  $t' - t'' - J_z$  model on the boundary between  $d$  and  $p$  symmetry, with a flat lower band in the pair excitation spectrum. In higher order,  $d$ -wave symmetry is selected from the lower pair band. However, we observe that the addition of the appropriate  $t' < 0$  and/or  $t'' > 0$ , the signs of  $t'$  and  $t''$  found in the hole-doped cuprates, could drive the hole-pair symmetry to  $p$ -wave, implying the possibility of competition between  $p$ -wave and  $d$ -wave pair ground states. (An added  $t' > 0$  and/or  $t'' < 0$  generally tend to promote  $d$ -wave symmetry.) We perturbatively construct an extended quasi-pair for the  $t - J_z$  model. In leading order, there are contributions from sites at a distance of  $\sqrt{2}$  lattice spacings apart; however, contributions from sites 2 lattice spacings apart, also of the same order, vanish identically. Finally, we compare our approach with analytic calculations for a  $2 \times 2$  plaquette and with existing numerical work, and discuss possible relevance to the physical parameter regime.

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## I. INTRODUCTION

In recent years a number of experiments, particularly phase-sensitive ones, have indicated that the pair symmetry of hole-doped cuprate superconductors is at least predominantly  $d_{x^2-y^2}$ <sup>1,2,3</sup>. Theoretical and numerical studies of the two-dimensional Hubbard,  $t - J$ , and related models have also suggested  $d_{x^2-y^2}$  pairing<sup>4,5,6,7,8,9</sup>, and studies of Hubbard and  $t - J$  models on  $2 \times 2$  plaquettes have provided an intuitive picture of how  $d$ -wave symmetry might arise<sup>10,11</sup>. However, there are few rigorous theoretical results in this general area.

Different experimental techniques have indicated that a pseudogap with the same symmetry as the superconducting gap persists above  $T_c$  in underdoped cuprates<sup>1,12,13,14,15,16</sup>. This, along with the short high- $T_c$  coherence length<sup>4</sup>, is qualitatively consistent with a strong-coupling picture, where pairs can preform at  $T > T_c$ <sup>17</sup>. Numerical work has in addition suggested that the  $t - J$  and  $t - J_z$  models have many similar properties<sup>4,18,19,20</sup> (see however Ref. 21), and that the  $t - J_z$  model may hence provide a suitable starting point for understanding  $t - J$  behavior<sup>22</sup>.

Reductions from CuO<sub>2</sub> three-band and similar models<sup>23</sup>, as well as comparison with ARPES results for a single doped hole<sup>24</sup>, suggest that, besides a nearest-neighbor (NN)  $t$ , the next-NN (NNN)  $t'$  and next-NNN (NNNN)  $t''$  hoppings may also be substantial. Numerical calculations and theory have explored some of the qualitative effect that the sign of  $t'$  has upon hole-pairing<sup>25,26,27</sup>. Given these above results, it is interesting to try to gain a better understanding of the pairing prop-

erties of the *extended*  $t - J$  model. In addition, performing such a study analytically could help provide guidance to future numerical work aimed at exploring specific regions of the model's phase diagram.

To that end, we consider in this paper two holes doped into the half-filled  $t - t' - t'' - J_z$  model in the strong coupling limit ( $J_z \gg |t|, |t'|, |t''|$ ). We calculate the symmetry of the hole pair in the ground state as well as the pair excitation spectrum. We do not explicitly consider the issues of phase separation or whether superconductivity actually occurs. We consider first the  $t' - J_z$  model, and show how singlet pairs can be constructed from our solutions. We next discuss the  $t' - t'' - J_z$  model, and then the  $t - J_z$  and  $t - t' - t'' - J_z$  models. For the  $t - J_z$  model, we perturbatively construct an extended quasi-pair. As a step towards exploring the range of validity of our approach, we compare with results for a  $2 \times 2$  plaquette and with numerical studies. Lastly, we discuss implications of our results for the physically relevant parameter regime, among which a phase competition scenario is one possibility.

Specifically, we consider the Hamiltonian

$$H = H_0 + H_1 + H_2 + H_3, \quad (1)$$

where

$$H_0 = J_z \sum_{x,y} \{ (S_{x,y}^z S_{x+1,y}^z + S_{x,y}^z S_{x,y+1}^z) - \frac{1}{4} (n_{x,y} n_{x+1,y} + n_{x,y} n_{x,y+1}) \}, \quad (2)$$

$$H_1 = (-t) \sum_{x,y,\sigma} \{ (\tilde{c}_{x,y,\sigma}^\dagger \tilde{c}_{x+1,y,\sigma} + H.c.) + (\tilde{c}_{x,y,\sigma}^\dagger \tilde{c}_{x,y+1,\sigma} + H.c.) \}, \quad (3)$$

$$H_2 = (-t') \sum_{x,y,\sigma} \{(\tilde{c}_{x,y,\sigma}^\dagger \tilde{c}_{x+1,y+1,\sigma} + H.c.) + (\tilde{c}_{x,y,\sigma}^\dagger \tilde{c}_{x+1,y-1,\sigma} + H.c.)\}, \quad (4)$$

and

$$H_3 = (-t'') \sum_{x,y,\sigma} \{(\tilde{c}_{x,y,\sigma}^\dagger \tilde{c}_{x+2,y,\sigma} + H.c.) + (\tilde{c}_{x,y,\sigma}^\dagger \tilde{c}_{x,y+2,\sigma} + H.c.)\}. \quad (5)$$

Here,  $x$  and  $y$  denote the coordinates of an  $L \times L$  lattice with periodic boundary conditions and even  $L$  (with, except for the  $t' - J_z$  model,  $L > 2$ ), and  $\sigma = \pm 1$  ( $\uparrow, \downarrow$ ) refers to electron spin.  $\tilde{c}_{x,y,\sigma} = c_{x,y,\sigma}(1 - n_{x,y,-\sigma})$ , enforcing the condition of no double occupancy.  $S_{x,y}^z = 1/2 (n_{x,y,\uparrow} - n_{x,y,\downarrow})$  and  $n_{x,y} = n_{x,y,\uparrow} + n_{x,y,\downarrow}$ . We do not explicitly consider here the spin-flip part of the magnetic interaction

$$H_\perp = \left(\frac{J_\perp}{2}\right) \sum_{x,y} \{(S_{x,y}^+ S_{x+1,y}^- + S_{x,y}^- S_{x,y+1}^+) + H.c.\}, \quad (6)$$

where  $S_{x,y}^+ = c_{x,y,\uparrow}^\dagger c_{x,y,\downarrow}$  and  $S_{x,y}^- = c_{x,y,\downarrow}^\dagger c_{x,y,\uparrow}$ . (The full  $t - t' - t'' - J$  model is recovered when  $J_\perp = J_z$ .)

At half filling each site is occupied by exactly one electron, and the doubly degenerate ground state of  $H_0$  is then that of a Néel antiferromagnet. We choose  $|\Phi_a\rangle$  to denote the state with electron spins  $\sigma(x,y) = (-1)^{x+y}$  and  $|\Phi_b\rangle$  to denote the state with  $\sigma(x,y) = (-1)^{x+y+1}$ . We define the operator  $a_{x,y} = c_{x,y,\sigma(x,y)}$  with  $\sigma(x,y) = (-1)^{x+y}$ , and the operator  $b_{x,y} = c_{x,y,\sigma(x,y)}$  with  $\sigma(x,y) = (-1)^{x+y+1}$ . Although our calculations and results are independent of the ordering convention chosen, we will denote for specificity

$$|\Phi_a\rangle = (a_{L,L}^\dagger \dots a_{1,L}^\dagger) \dots (a_{L,2}^\dagger \dots a_{1,2}^\dagger) (a_{L,1}^\dagger \dots a_{1,1}^\dagger) |0\rangle, \quad (7)$$

where  $|0\rangle$  is the state with no electrons, with an analogous definition for  $|\Phi_b\rangle$ .

We now dope the half-filled state  $|\Phi_a\rangle$  with two holes and consider the strong-coupling limit ( $J_z \gg |t|, |t'|, |t''|$ ). In this limit, there will be an energy cost of order  $J_z$  if the two holes are *not* NN. Hence, to zeroth order, the (highly degenerate) two-hole ground state is spanned by the set of all NN hole pairs. We denote the state with a horizontal NN hole pair at sites  $(x,y)$  and  $(x+1,y)$  as

$$|h_{x,y}\rangle = a_{x+1,y} a_{x,y} |\Phi_a\rangle, \quad (8)$$

and the state with a vertical NN hole pair at sites  $(x,y)$  and  $(x,y+1)$

$$|v_{x,y}\rangle = a_{x,y+1} a_{x,y} |\Phi_a\rangle. \quad (9)$$

The  $|h_{x,y}\rangle$ 's and  $|v_{x,y}\rangle$ 's provide a complete, orthonormal basis for the two-hole ground state of  $H_0$  corresponding to  $|\Phi_a\rangle$ .

It costs an energy of order  $J_z$  if one of the NN holes hops to a NN site through the hybridization matrix element  $t$ . However, there is no energy cost for hops corresponding to  $t'$  or  $t''$ , as long as the two holes remain NN

after the hop. Thus, to lowest order in  $1/J_z$ , it is only necessary to diagonalize the Hamiltonian  $H_2 + H_3$  in the subspace spanned by the  $|h_{x,y}\rangle$ 's and  $|v_{x,y}\rangle$ 's; i.e., it is only necessary to consider the  $t' - t'' - J_z$  model. We note that in this limit the  $t' - t'' - J_z$  model becomes isomorphic to the strong-coupling limit of the antiferromagnetic van Hove model of ref. 28.

## II. $t' - J_z$ MODEL

We consider first the  $t' - J_z$  model, involving only the  $H_2$  (diagonal) hopping term. Defining

$$|h_{k_x,k_y}\rangle = \frac{1}{L} \sum_{x,y} e^{-\frac{2\pi i k_x x}{L}} e^{-\frac{2\pi i k_y y}{L}} |h_{x,y}\rangle \quad (10)$$

and

$$|v_{k_x,k_y}\rangle = \frac{1}{L} \sum_{x,y} e^{-\frac{2\pi i k_x x}{L}} e^{-\frac{2\pi i k_y y}{L}} |v_{x,y}\rangle, \quad (11)$$

with  $k_x, k_y = 0, 1 \dots L-1$ , we obtain the lowest order wave functions

$$|\psi_{k_x,k_y}^\pm\rangle = \frac{1}{\sqrt{2}} \left\{ e^{-\frac{\pi i k_x x}{L}} |h_{k_x,k_y}\rangle \pm \text{sgn}(t') e^{-\frac{\pi i k_y y}{L}} |v_{k_x,k_y}\rangle \right\} \quad (12)$$

with energies

$$\epsilon_{k_x,k_y}^\pm = \pm 4|t'| \sin\left(\frac{\pi k_x}{L}\right) \sin\left(\frac{\pi k_y}{L}\right). \quad (13)$$

Since  $0 \leq \sin(\pi k_x/L), \sin(\pi k_y/L) \leq 1$ , the minus sign gives the branch of lower energy. The lowest energy state  $|\psi_0^{(a)}\rangle$ , with energy  $-4|t'|$ , occurs when  $k_x = L/2$  and  $k_y = L/2$  (i.e.,  $(\pi, \pi)$ ). Rewriting in terms of the  $a_{x,y}$ 's and neglecting overall phase factors, one obtains

$$|\psi_0^{(a)}\rangle = \frac{1}{L\sqrt{2}} \sum_{x,y} (-1)^{x+y} \{a_{x+1,y} a_{x,y} - \text{sgn}(t') a_{x,y+1} a_{x,y}\} |\Phi_a\rangle \quad (14)$$

When  $t' > 0$  ( $\text{sgn}(t') = 1$ ), the sum over hole pair operators in Eq. 14 changes sign upon a 90 degree rotation around a lattice point, giving the pair  $d$ -wave symmetry (specifically,  $d_{x^2-y^2}$ <sup>2,3,7</sup>). When  $t' < 0$ , there are no such sign changes, giving  $s$ -wave symmetry (specifically, extended- $s$ <sup>2,7</sup>).

If one adds to Eq. 14 the appropriately-phased pair operator for two holes doped into the ground state  $|\Phi_b\rangle$ , given in

$$|\psi_0^{(b)}\rangle = \frac{1}{L\sqrt{2}} \sum_{x,y} (-1)^{x+y+1} \{b_{x+1,y} b_{x,y} - \text{sgn}(t') b_{x,y+1} b_{x,y}\} |\Phi_b\rangle, \quad (15)$$

one obtains for  $t' > 0$  the usual NN singlet  $d_{x^2-y^2}$  pair operator

$$\Delta_d = \frac{1}{2L} \sum_{x,y} \left\{ (c_{x,y,\uparrow} c_{x+1,y,\downarrow} - c_{x,y,\downarrow} c_{x+1,y,\uparrow}) - (c_{x,y,\uparrow} c_{x,y+1,\downarrow} - c_{x,y,\downarrow} c_{x,y+1,\uparrow}) \right\}, \quad (16)$$

with  $t' < 0$  giving the analogous singlet extended- $s$  operator

$$\Delta_s = \frac{1}{2L} \sum_{x,y} \left\{ (c_{x,y,\uparrow} c_{x+1,y,\downarrow} - c_{x,y,\downarrow} c_{x+1,y,\uparrow}) + (c_{x,y,\uparrow} c_{x,y+1,\downarrow} - c_{x,y,\downarrow} c_{x,y+1,\uparrow}) \right\}. \quad (17)$$

With different relative phases, one can also obtain types of  $d$ -wave or  $s$ -wave  $m = 0$  triplet pairs; because quantum spin fluctuations are not included in the  $t - J_z$  model, the cases cannot be differentiated at this level.

One can better understand the dependence of the  $t' - J_z$  (and  $t' - J$ ) pair symmetry on  $\text{sgn}(t')$  by considering phase transformations of electron creation and destruction operators. Specifically, we consider transformations of the form  $c_j = e^{i\theta(j)} d_j$ , where  $j$  is some generalized coordinate referring to both orbital and spin and  $\theta(j)$  is some function of  $j$ .

First, as background, let  $P$  denote some arbitrary product of electron creation and destruction operators, some of which operators may be the same, with coordinates referring to orthogonal states. For example, for a one-dimensional chain with one orbital per site, one could have  $P = c_{1\uparrow}^\dagger c_{4\downarrow}^\dagger c_{1\uparrow} c_{2\downarrow}^\dagger c_{1\uparrow}^\dagger$ .

As previously, let  $|0\rangle$  denote a state with no electrons. Then,  $\langle 0|P^\dagger P|0\rangle$  if it is nonzero reduces to

$$\langle 0|P^\dagger P|0\rangle = \langle 0|\prod_{\{j\}} c_j c_j^\dagger|0\rangle = \langle 0|\prod_{\{j\}} (1 - n_j)|0\rangle \quad (18)$$

for some subset  $\{j\}$  of the generalized  $j$  coordinates. Hence, any phase transformation of the form  $c_j = e^{i\theta(j)} d_j$  does not affect the value of  $\langle 0|P^\dagger P|0\rangle$ .

Now, consider  $\langle 0|P_l^\dagger P_{l'}|0\rangle$ , where  $P_l$  and  $P_{l'}$  are two different products of creation and destruction operators. Each nonzero  $\langle 0|P_l^\dagger P_{l'}|0\rangle$  also reduces to the general form  $\langle 0|\prod_{\{j\}} c_j c_j^\dagger|0\rangle$ , which is again unaffected by the transformations  $c_j = e^{i\theta(j)} d_j$ . Lastly, consider the expectation value of an operator  $O = \sum_l a_l P_l$  in the (possibly unnormalized) state  $\sum_l b_l P_l|0\rangle$ , where the  $a_l$  and  $b_l$  are coefficients. Then,

$$\begin{aligned} \langle O \rangle &= \frac{\langle 0|\sum_l b_l^* P_l^\dagger O \sum_{l'} b_{l'} P_{l'}|0\rangle}{\langle 0|\sum_l b_l^* P_l^\dagger \sum_{l'} b_{l'} P_{l'}|0\rangle} \\ &= \frac{\sum_{l,l'} a_{l'} b_{l'}^* \langle 0|P_l^\dagger P_{l'} P_{l'}|0\rangle}{\sum_{l,l'} b_l^* b_{l'} \langle 0|P_l^\dagger P_{l'}|0\rangle}. \end{aligned} \quad (19)$$

Again, each term of the numerator and denominator reduces to the form  $\langle 0|\prod_{\{j\}} c_j c_j^\dagger|0\rangle$ , which is invariant under  $c_j = e^{i\theta(j)} d_j$ . Hence, an arbitrary phase transformation on electron creation and destruction operators has no effect on fermion operator expectation values in fermion states. Also, since an electron creation/destruction operator referring to a particular basis can always be written as a sum of operators referring to a different orthogonal basis, it is not even necessary that the creation/destruction operators under consideration refer to a particular orthogonal basis, as long as the phase transformations are consistent.

Now, we wish to find a particular phase transformation which is equivalent to reversing the sign of  $t'$ . Temporarily dropping the spin coordinate, we choose for simplicity a transformation of the form

$$c_{x,y} = e^{i(\phi_x x + \phi_y y)} d_{x,y}, \quad (20)$$

where  $\phi_x$  and  $\phi_y$  are constants. (We do not include a constant phase factor as it has no relevant effect.) We require:

$$c_{x+1,y+1}^\dagger c_{x,y} + H.c. = (-1)[d_{x+1,y+1}^\dagger d_{x,y} + H.c.] \quad (21)$$

and

$$c_{x-1,y+1}^\dagger c_{x,y} + H.c. = (-1)[d_{x-1,y+1}^\dagger d_{x,y} + H.c.]. \quad (22)$$

Solving the previous equations, one can obtain

$$\phi_x + \phi_y = (2p + 1)\pi \quad (23)$$

and

$$\phi_x - \phi_y = (2q + 1)\pi \quad (24)$$

for arbitrary integers  $p$  and  $q$ , of which solutions are

$$c_{x,y} = (-1)^x d_{x,y}, \quad (25)$$

or

$$c_{x,y} = (-1)^y d_{x,y}. \quad (26)$$

Restoring the spin coordinates leads to the four following transformations equivalent to changing the sign of  $t'$ :

$$c_{x,y,\uparrow} = (-1)^x d_{x,y,\uparrow}, \quad c_{x,y,\downarrow} = (-1)^x d_{x,y,\downarrow}; \quad (27)$$

$$c_{x,y,\uparrow} = (-1)^y d_{x,y,\uparrow}, \quad c_{x,y,\downarrow} = (-1)^y d_{x,y,\downarrow}; \quad (28)$$

$$c_{x,y,\uparrow} = (-1)^x d_{x,y,\uparrow}, \quad c_{x,y,\downarrow} = (-1)^y d_{x,y,\downarrow}; \quad (29)$$

$$c_{x,y,\uparrow} = (-1)^y d_{x,y,\uparrow}, \quad c_{x,y,\downarrow} = (-1)^x d_{x,y,\downarrow}. \quad (30)$$

None of the above four transformations changes the sign of the  $J_z$  term (Eq. 2). However, the transformations of Eqs. 29 and 30 (as well as more general transformations not discussed here which are different on different sublattices) do not leave the  $H_\perp$  of Eq. 6, and

hence the spin-spin interaction of the  $t' - J$  model, invariant. The transformations of Eqs. 27 and 28, which do leave  $H_\perp$  invariant, change the  $d_{x^2-y^2}$  symmetry of the pairs of Eq. 14 to  $s$  and the  $d_{x^2-y^2}$  singlet pairs of Eq. 16 to extended- $s$  singlets and vice-versa. Hence,  $d_{x^2-y^2}$  singlets of the form of Eq. 16 are transformed to extended- $s$  singlets when the sign of  $t'$  is changed in the  $t' - J$  model, and vice-versa. More generally, operators are transformed according to Eq. 27 or 28 when the sign of  $t'$  is changed. (The two transformations give the same results for operators with the appropriate symmetries, which generally includes the operators of interest). This is different from ref. 27. However, the main arguments and conclusions of that paper remain unchanged.

### III. $t' - t'' - J_z$ MODEL

For the more general  $t' - t'' - J_z$  model, one obtains in lowest order the (unnormalized) wave functions

$$|\psi_{k_x, k_y}^\pm\rangle = e^{-\frac{\pi i k_x x}{L}} (4t') s_x s_y |h_{k_x, k_y}\rangle + e^{-\frac{\pi i k_y y}{L}} \left[ (2t'')(s_y^2 - s_x^2) \pm \tau_{x,y} \right] |v_{k_x, k_y}\rangle \quad (31)$$

with energies

$$\epsilon_{k_x, k_y}^\pm = (-2t'')(1 - s_x^2 - s_y^2) \pm \tau_{x,y}, \quad (32)$$

where  $s_x = \sin(\pi k_x/L)$ ,  $s_y = \sin(\pi k_y/L)$ , and

$$\tau_{x,y} = 2 \left\{ (t'')^2 (s_x^2 - s_y^2)^2 + 4(t')^2 s_x^2 s_y^2 \right\}^{\frac{1}{2}}. \quad (33)$$

As a function of  $t'$  and  $t''$ , we find that the ground state symmetry of the pair is as shown in Fig. 1.

The  $s$ -wave and  $d$ -wave operators are of the form in Eq. 14. The ground state associated with  $p$ -wave pairs is, in contrast, highly degenerate. The multiple  $p$ -wave pair operators can be either  $p_x$

$$\Delta_{p_x}(k_y) = \frac{1}{L\sqrt{2}} \sum_{x,y} e^{-\frac{2\pi i k_y y}{L}} a_{x,y} (a_{x+1,y} - a_{x-1,y}) \quad (34)$$

or  $p_y$

$$\Delta_{p_y}(k_x) = \frac{1}{L\sqrt{2}} \sum_{x,y} e^{-\frac{2\pi i k_x x}{L}} a_{x,y} (a_{x,y+1} - a_{x,y-1}). \quad (35)$$

In leading order, the  $p_x$  states have energies independent of  $k_y$ , and the  $p_y$  states have energies independent of  $k_x$ . Both  $p$ -wave pair operators change sign under a 180 degree rotation.

### IV. $t - J_z$ MODEL

We next consider the strong-coupling limit of the  $t - J_z$  model. To lowest order, we find that this maps onto the

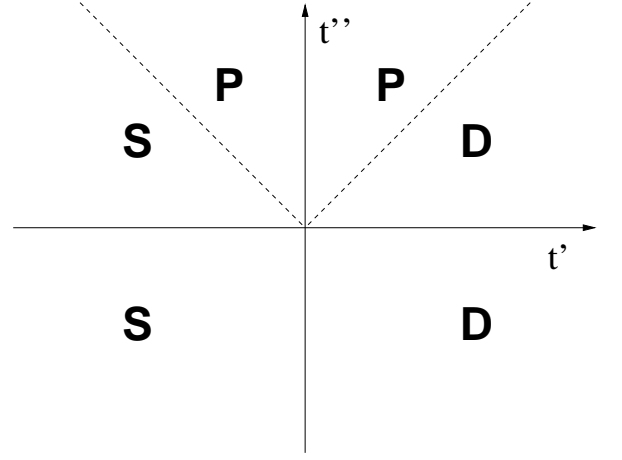


FIG. 1: Hole pair symmetry in the strong-coupling limit of the  $t' - t'' - J_z$  model as a function of  $t'$  and  $t''$ . The legend is as follows: “D” denotes  $d_{x^2-y^2}$ , “P” denotes  $p_x$  or  $p_y$ , and “S” denotes extended- $s$ . The axes cross at  $t' = 0$  and  $t'' = 0$ .

above strong-coupling limit of the  $t' - t'' - J_z$  model with

$$t'_{t,eff.} = t''_{t,eff.} = \frac{2}{3} \left( \frac{t^2}{J_z} \right). \quad (36)$$

From Eq. 32, the lower band of the pair excitation spectrum then becomes flat, with wave functions

$$|\psi_{k_x, k_y}^-\rangle = \frac{1}{\sqrt{2}} \left\{ e^{-\frac{\pi i k_x x}{L}} s_y |h_{k_x, k_y}\rangle - e^{-\frac{\pi i k_y y}{L}} s_x |v_{k_x, k_y}\rangle \right\}. \quad (37)$$

Flat pair bands were also found<sup>29,30</sup> for related (though different) models and/or treatments. In ref. 22, a five-fold degeneracy of strong-coupling  $t - J_z$  pairs of pure  $d$  or  $p$  symmetry was noted.

We see from Eq. 36 that, to lowest order, the strong-coupling  $t - J_z$  model lies on the (rightmost) boundary in Fig. 1 between  $d$ -wave and  $p$ -wave symmetry, providing a simple picture for competition between these two states. In the next higher order, neglecting constant additive terms, the energies of the lower pair band separate into

$$\epsilon_{k_x, k_y}^- = \left( -\frac{8}{45} \right) \left( \frac{t^4}{J_z^3} \right) \left( 2 - c_x - c_y \right)^{-1} \{ c_x^2 + c_y^2 + 4c_x c_y - 31c_x - 31c_y + 56 \}, \quad (38)$$

where here  $c_x = \cos(2\pi k_x/L)$  and  $c_y = \cos(2\pi k_y/L)$ . Two-hole lower band dispersion curves were previously calculated numerically using a variational method<sup>31</sup> and series expansions<sup>20</sup>. We then find (in agreement with refs. 20 and 22) that the pure  $d$ -wave ( $t' > 0$ ) state of Eq. 14 is selected as the lower pair band ground state. However, the closeness to  $p$ -wave symmetry may provide an explanation for the low-energy  $p$ -wave “quasi-pair” peaks seen numerically in small  $t - J$  and  $t - J_z$  clusters<sup>18</sup>.

We also note that several different techniques have suggested that the symmetry of a doped hole pair in the

$t - J_z$  and/or  $t - J$  models may be  $p$ -wave for some range of generally intermediate or small  $J_z/t$  or  $J/t$ <sup>20,31,32,33</sup>. However, this has not been rigorously confirmed one way or the other<sup>34,35</sup>.

One can perturbatively construct increasingly extended quasi-pair states for the  $t - J_z$  model. Combining results for the NN  $d$ -wave pair operators for ground states  $|\Phi_a\rangle$  and  $|\Phi_b\rangle$ , one finds the lowest order correction for the singlet pair operator of Eq. 16

$$\Delta'_d = \left(-\frac{2}{3}\right) \left(\frac{t}{J_z}\right) \left(\frac{1}{L}\right) \sum_{x,y,\sigma} \sigma \left\{ \begin{aligned} & (c_{x+1,y,\sigma}^\dagger c_{x+1,y,-\sigma} - c_{x,y+1,-\sigma}^\dagger c_{x,y+1,\sigma}) \\ & c_{x+1,y+1,\sigma} c_{x,y,\sigma} \\ & + (c_{x+1,y,\sigma}^\dagger c_{x+1,y,-\sigma} - c_{x,y-1,-\sigma}^\dagger c_{x,y-1,\sigma}) \\ & c_{x+1,y-1,\sigma} c_{x,y,\sigma} \end{aligned} \right\}. \quad (39)$$

When operating on the appropriate Néel state, each of the above terms consists of a diagonal hole pair “dressed” with a singlet pair of electrons straddling the bond connecting the pair of holes, as was found in numerical  $t - J$  simulations<sup>11</sup>. This form basically arises from the disruption in the local spin order when an electron of particular spin orientation and one hole of a NN hole pair exchange sites to form a diagonal hole pair. We note that the contribution from pairs a distance of two lattice sites apart, nominally also of order  $t/J_z$ , vanishes identically in this order. (Variational calculations found a reduction of such a contribution<sup>36</sup>.) This vanishing may provide an explanation for why only NN and diagonal hole correlations appear to dominate in the  $t - J$  model near half filling for moderate to large  $J/t$ <sup>11,37</sup>.

If one adds the necessary terms to the operator of Eq. 39 to impose a type of spin rotational invariance, one obtains the composite pair operator invented in ref. 37 to give a diagonal singlet pair with  $d_{x^2-y^2}$  symmetry. The type of operator of ref. 37 was also generated<sup>11</sup> in a  $2 \times 2$  plaquette by applying  $e^{-\tau H}$  to the pair operator of Eq. 16. The operator of Eq. 39, which emerges naturally from perturbation theory, also has  $d_{x^2-y^2}$  symmetry.

We also note that, since we calculate energy spectra and wave functions, our results and approach can be used to calculate finite-temperature and real frequency properties. Our results can also be easily extended to periodic  $n$ -leg ladders with even  $n$ . However, we do not pursue those issues here.

We in addition note that, in contrast to Eqs. 27 through 30, the phase transformation that is equivalent to changing the sign of  $t$  is given by

$$d_{x,y,\sigma} = (-1)^{x+y} c_{x,y,\sigma}. \quad (40)$$

This transformation leaves the spin-spin interactions  $H_0$  and the  $H_\perp$  of Eq. 6 invariant. Under this transformation the symmetries of the hole pair operators of Eqs. 14, 16, and 39 all remain the same.

## V. $t - t' - t'' - J_z$ MODEL AND INTERMEDIATE COUPLING

For  $|t|, |t'|, |t''| \ll J_z$ ;  $|t| \gg |t'|, |t''|$ ; and  $|t'/J_z| \gg (t/J_z)^4$  or  $|t''/J_z| \gg (t/J_z)^4$  (so that lowest order terms dominate), one can use Eq. 36 to define a

$$t'_{eff.} = t' + t'_{t,eff.} = t' + \frac{2}{3} \frac{t^2}{J_z} \quad (41)$$

and

$$t''_{eff.} = t'' + t''_{t,eff.} = t'' + \frac{2}{3} \frac{t^2}{J_z}. \quad (42)$$

One can then simply use Fig. 1 as a guide to pair symmetry.

As one step towards investigating the further range of validity of our approach, we performed analytic calculations of the  $t - t' - J_z - J_\perp$  model (see Eq. 6) on a  $2 \times 2$  plaquette. In what follows, the four plaquette sites are consecutively numbered as one goes around the plaquette edge. Spin-spin interactions and  $t$  hoppings are between consecutive sites,  $t'$  hoppings are between diagonal sites, and there are *no* periodic boundary conditions (though such boundary conditions would only renormalize parameter values).

With no holes (four electrons, one per site), we found that the ground state had  $d_{x^2-y^2}$  symmetry, as is the case for the  $t - J$  model on a plaquette<sup>10,11</sup>, for all  $J_z > 0$ ,  $J_\perp \geq 0$ . (There are two degenerate states only when  $J_\perp = 0$ , both of  $d$ -wave symmetry).

For two holes, when

$$t' > t'_{cross.} = \frac{1}{8} [(J_z + J_\perp) - \sqrt{(J_z + J_\perp)^2 + 64t^2}] \quad (43)$$

(the more “physical” parameter regime), the ground state energy is

$$E_0 = -\frac{1}{2} [\alpha + (\alpha^2 + 32t^2)^{\frac{1}{2}}], \quad (44)$$

where

$$\alpha = \frac{J_z}{2} + \frac{J_\perp}{2} + 2t'. \quad (45)$$

(We assume  $J_z > 0$ ,  $J_\perp \geq 0$ , and either  $t \neq 0$  or  $t' \neq 0$ ). Defining<sup>11</sup>

$$\Delta_{ij}^\dagger = \frac{1}{\sqrt{2}} (c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger - c_{i\downarrow}^\dagger c_{j\uparrow}^\dagger) \quad (46)$$

with  $\Delta_{ij}^\dagger = \Delta_{ji}^\dagger$ , where  $i$  and  $j$  refer to plaquette sites, the ground state is a linear combination of the two states

$$|\psi_1\rangle = \frac{1}{\sqrt{2}} (\Delta_{13}^\dagger + \Delta_{24}^\dagger) |0\rangle \quad (47)$$

and

$$|\psi_2\rangle = \frac{1}{2} (\Delta_{12}^\dagger + \Delta_{23}^\dagger + \Delta_{34}^\dagger + \Delta_{41}^\dagger) |0\rangle. \quad (48)$$

The ground state hence has  $s$ -wave symmetry, as was earlier found for the two-hole doped plaquette  $t - J$  model<sup>10,11</sup>. As discussed previously<sup>10,11</sup>, this implies that the hole pair symmetry is  $d$ -wave. We note that with  $t' = 0$ , which automatically satisfies Eq. 43, the hole pair symmetry for the plaquette  $t - J_z - J_\perp$  model is always  $d$ -wave, as in the strong-coupling limit of the general  $t - J_z$  model. (However, because there are no lattice sites a distance of two lattice spacings apart on the plaquette, for  $t/J_z \ll 1$  the plaquette  $t - J_z$  model reduces to a  $t' - J_z$  model with  $t' > 0$  rather than a full  $t' - t'' - J_z$  model, enhancing  $d$ -wave pairing compared to a larger lattice.)

However, there is a level crossing at  $t' = t'_{cross.}$ , and when  $t' < t'_{cross.}$  the ground state has energy

$$E_0 = -\frac{J_z}{2} - \frac{J_\perp}{2} + 2t' \quad (49)$$

and wave function

$$|\psi_3\rangle = \frac{1}{2}(\Delta_{12}^\dagger - \Delta_{23}^\dagger + \Delta_{34}^\dagger - \Delta_{41}^\dagger)|0\rangle. \quad (50)$$

$|\psi_3\rangle$  has  $d$ -wave symmetry, implying that the hole pair symmetry is now  $s$ -wave. We note that with  $t = 0$ , giving  $t'_{cross.} = 0$ , the  $t' - J_z - J_\perp$  model hole pair symmetry on a plaquette is  $d$ -wave for  $t' > 0$  and  $s$ -wave for  $t' < 0$ , as in the general  $t' - J_z$  model strong coupling case.

As mentioned previously, some approaches have suggested  $p$ -wave hole-pair symmetry for some range of generally intermediate or small  $J/t$  or  $J_z/t$ <sup>20,31,32,33</sup>. However, other  $t - J$  numerical results<sup>22,34,35,37</sup> indicate that  $d$ -wave features of the strong-coupling limit may persist down to physically relevant intermediate coupling ( $J/t \approx 0.3 - 0.5$ ). This and the above plaquette results are consistent with the strong-coupling  $t - t' - t'' - J_z$  model as a potentially useful starting point to explore the more physically relevant intermediate-coupling  $t - t' - t'' - J$  model.

As a rough guide to the general effects of  $t'$  and  $t''$  on pairing symmetry, one can begin with a  $d$ -wave state in Fig. 1 arising from the  $t$  term, presumably in the upper right quadrant. Assuming pairs of pure symmetry and that strong coupling qualitatively extends to  $|t'|, |t''| \sim J, J_z$ , both  $t' > 0$  and  $t'' < 0$  will tend to move one deeper into the  $d$ -wave region; however,  $t' < 0$  and  $t'' > 0$  will tend to move one towards, and perhaps into, the  $p$ -wave region. Previous  $t - J$  work has argued and/or indicated numerically that  $t' > 0$  strengthens  $d$ -wave pairing while  $t' < 0$  weakens it<sup>26,27</sup>, and it was found on a 32-site lattice that a particular  $t' < 0$  and  $t'' > 0$  together favored a  $p$ -wave pair<sup>33</sup>. Also, if one starts with a possible  $t - J_z$  or  $t - J$   $p$ -wave pair (upper right quadrant),  $t' < 0$  and  $t'' > 0$  would tend to move one deeper into the  $p$ -wave region while  $t' > 0$  and  $t'' < 0$  would tend to move one toward, and perhaps even into, the  $d$ -wave region.

Based on this and our strong-coupling results (assuming pairs of pure symmetry), we show in Fig. 2 qualitative predictions of the hole pair symmetry for the  $t - t' - J_z$

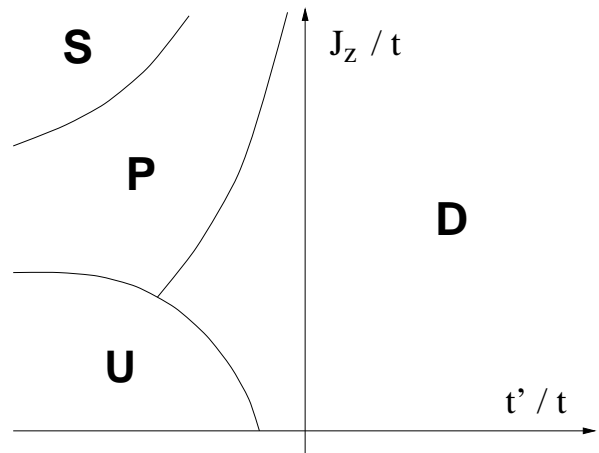


FIG. 2: Qualitative diagram of proposed hole pair symmetry for the  $t - t' - J_z$  model. “D”, “P”, and “S” denote the same as in Fig. 1, and no prediction is made for region “U”. Axes cross at  $t'/t = 0$  and intermediate  $J_z/t$  ( $\sim 0.3 - 0.5$ ). The possibility of  $p$ -wave symmetry for  $t' = 0$  and intermediate  $J_z/t$  is not shown.

model. We do not show in Fig. 2 the possibility of a cross-over to  $p$ -wave symmetry for the  $t - J_z$  model mentioned above. We believe the predictions shown apply to the  $t - t' - J$  model as well, with a comparatively smaller  $p$ -wave region due to larger energy differences between  $t - J$   $p$ -wave and  $d$ -wave pair states<sup>18</sup>. An additional  $t'' > 0$  would tend to enlarge the  $p$ -wave region, and an additional  $t'' < 0$  would tend to enlarge the  $d$ -wave region. Note that in Fig. 2, the horizontal axis cuts the vertical axis at intermediate  $J_z/t$  ( $\sim 0.3 - 0.5$ ).

$t > 0$  for the hole-doped cuprates, and estimates for  $t'$  and  $t''$  are typically in the ranges  $t' \approx (-0.1)t - (-0.5)t$ , and  $t'' \approx 0.0 - (0.3)t$ , generally with  $|t'| > |t''|$ <sup>23,24</sup>. Both these signs of  $t'$  and  $t''$  are those which could tend to drive the pair symmetry to  $p$ -wave, raising the issue of the hole pair symmetry in the intermediate-coupling regime. We note that  $s$ -wave is also possible, though we believe it less likely at intermediate coupling.

It would be interesting to try to determine numerically whether the symmetry of two doped holes in the  $t - t' - t'' - J$  model is in fact  $d$ -wave for the experimentally relevant values of  $t, t', t''$ , and  $J$  (e.g.,  $J/t \approx 0.3 - 0.5$ ). However, drawing conclusions from exact diagonalization and other current approaches may be challenging (see, e.g., refs. 25 and 33) due to the possibility of uncontrolled finite-size or other errors, and such approaches sometimes give conflicting results. If the symmetry were established to be  $p$ -wave rather than  $d$ -wave, it would suggest that the  $t - t' - t'' - J$  model by itself could be incomplete as a model for high- $T_c$  superconductivity. In that case, one possibility for restoring  $d$ -wave symmetry could be the addition of electron-phonon coupling in the  $d$ -channel<sup>38</sup>. In either case, it may also be of interest to explore how the existence of or nearness to  $p$ -wave symmetry, which effectively reduces the dimensionality of the

hole pair wave function from 2D to 1D, would correlate with possible stripe phases observed experimentally<sup>39,40</sup> and in numerical simulations<sup>41,42,43</sup>.

Another interesting possibility is the existence of a novel exotic state which may be close in energy to the  $d_{x^2-y^2}$  superconducting cuprate ground state. Such a *competing phases* scenario<sup>44</sup> could become even more involved if one takes in account recent numerical calculations<sup>45</sup> pointing to the existence of strong ferromagnetic fluctuations in the vicinity of doped holes for realistic values of  $t' < 0$ .

## VI. SUMMARY

In summary, we have investigated analytically the ground state pair symmetry and excitation spectra of two holes doped into the half-filled  $t - t' - t'' - J_z$  model in the strong-coupling limit. In lowest order, this reduces to considering the  $t' - t'' - J_z$  model, where we found regions of ground state  $d$ -wave,  $s$ -wave, and (degenerate)  $p$ -wave symmetry, depending upon the signs and relative magnitudes of  $t'$  and  $t''$ . We next found that the  $t - J_z$  model in lowest order was on the boundary between  $d$ -wave and  $p$ -wave pair symmetry, with a flat lower pair dispersion, providing a simple picture for the competition between  $d$  and  $p$  symmetries. In higher order,  $d$ -wave symmetry was selected from the lower pair band. However, because of the closeness to  $p$ -wave symmetry, we predict that the appropriate  $t' < 0$  and/or  $t'' > 0$  added to the  $t - J_z$  or  $t - J$  models with intermediate to large  $J_z$  or  $J$  should drive them into  $p$ -wave pairs, and perhaps even  $p$ -wave super-

conductivity. These signs of  $t'$  and  $t''$  are those found in the hole-doped cuprates. (In contrast,  $t' > 0$  and/or  $t'' < 0$  tend to promote  $d$ -wave symmetry.) This  $p$ -wave tendency could be strengthened following results which suggest  $p$ -wave pair symmetry for intermediate or small  $J/t$  or  $J_z/t$  in the  $t - J$  or  $t - J_z$  models<sup>20,31,32,33</sup>, though such results have not been rigorously confirmed<sup>34,35</sup>.

We constructed a perturbative correction to the nearest-neighbor  $d$ -wave pair, giving a more extended quasi-pair, and found that it was similar to the  $d$ -wave composite operator invented in ref. 37 and qualitatively consistent with previous numerical results<sup>11</sup>. The quasi-pair included a contribution from sites  $\sqrt{2}$  lattice spacings apart, but the same-order contribution from sites 2 lattice spacings apart vanished identically. The structure of the quasi-pair derived from the disruption in local spin order under the exchange of one of the nearest neighbor holes and an electron.

We explored ranges of validity of the perturbative approach of this paper using a  $2 \times 2$  plaquette and results from other work<sup>22,34,35,37</sup>. Lastly, we discussed implications for the experimentally relevant parameter regime. These included the possibility of  $p$ -wave symmetry for two doped holes, which would suggest that the  $t - t' - t'' - J$  model could be incomplete as a high- $T_c$  model, or perhaps a phase competition scenario between  $d$ -wave superconductivity and a  $p$ -wave state.

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